



Ion Composition Elucidation (ICE): a High Resolution Mass Spectrometric Technique for Identifying Compounds in Complex Mixtures

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Three Compound Identification Problems

1. Multiple Plausible Library Matches

The mass spectrum in Figure 1a is a background-subtracted mass spectrum for a compound in an extract of 12 L of effluent from a tertiary waste water treatment plant. Figures 1b-g are NIST library matches over the same mass range. The isomers in parenthesis in Figure 1 also had similar NIST mass spectra. The compound that provided the mass spectrum was present in the extract at an ultra-trace level. Chemical noise, coelution of compounds in the complex extract, and septum and column bleed components generally result in background-subtracted mass spectra containing extraneous ions or lacking low-abundance ions expected from the analyte. Hence, none of the NIST library matches can be ruled out without additional data.

